B.2. SCATTERING THEORY

Scattering theory is a refined example of perturbation theory, adapted to a particular set of boundary conditions (incoming waves incident on a central potential). The practical importance for particle physics experiments, as well as collision theory in many-body systems, led to a very sophisticated development of this theory in the period 1930s - 1960s. The purpose of this section is (a) introductory - to give you a door into the subject (about which many books have been written), and (b) pedagogical - to see how the basic structure of perturbative expansions works.

B.2.1. BASIC FORMULATION

Scattering theory can of course be developed for a many-particle system, but here, as always in this course, we are only interested in 1- or 2-particle systems. The scattering problem for 2 particles can always be reduced to a 1-particle problem in the absence of an external potential, so we will be concerned here with the scattering of a single particle off some potential. In what follows we first formulate the problem and the method as a special case of time-independent perturbation theory, in terms of the propagator for the scattering particle. Then we look at the detailed properties of the scattering function (which is related very simply to the propagator - it is the amplitude to go from the initial plane wave state to some final scattered state).

B.2.1.(a) PROPAGATOR : PERTURBATION THEORY

As is often the case, the best way to formulate this from the beginning is using path integral theory. We assume a Hamiltonian of form

$$\mathcal{H} = \mathcal{H}_0 + V(t) \tag{182}$$

and immediately specialise to the case: $V(t) = V = \text{const}$ (183)

The time-dependent case is dealt with later. Now let us assume we already know the propagator G_0 for the Hamiltonian $\mathcal{H}_0$; we want an expression for the propagator $\mathbf{G}$ for the full problem. We have

$$G_0(\beta,\alpha;t,t') = \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{i/\hbar \int_{t'}^{t} d\tau\, L_0(x,\dot{x})} \tag{184}$$

in an obvious notation where α, β denote states $|\alpha\rangle, |\beta\rangle$, and we project onto these initial and final states. It then follows that

$$\left.\begin{aligned} \mathbf{G}_{\beta\alpha}(\{V\};t) &= \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{i/\hbar \int_{t'}^{t} d\tau\, (L_0(x,\dot{x}) - V(x,\dot{x}))} \\ &= \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{i/\hbar \int d\tau\, L_0(x,\dot{x})} \sum_{k=0}^{\infty} \left(-\frac{i}{\hbar}\right)^k \frac{1}{k!} \left(\int_{t'}^{t} d\tau\, V(x(\tau))\right)^k \end{aligned}\right\} \tag{185}$$

$$\equiv \sum_{k=0}^{\infty} \tilde{\mathcal{G}}_k^{\beta\alpha}(t) \tag{186}$$

One can write an obvious integral eqtn for this Green fn., by noting that

$$\left.\begin{aligned}\bar{\mathcal{G}}_k^{\beta\alpha}(t,t') &= \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{\frac{i}{\hbar}\int_{t'}^{t} d\tau\, L_0(x\dot{x})} \left(\frac{-i}{\hbar}\right)^k \prod_{r=0}^{k} \int d\tau_r \; V(x(\tau_r)) \\ &\equiv \int_\alpha^\beta \mathcal{D}x\, e^{\frac{i}{\hbar}\int_{t'}^{t} L_0(x,\dot{x})} \int_{t'}^{t} d\tau_k \int_{t'}^{\tau_k} d\tau_{k-1} \cdots \int_{t'}^{\tau_2} d\tau_1 \left(\frac{-i}{\hbar}\right)^k V(x(\tau_k))\, V(x(\tau_{k-1}))\cdots V(x(\tau_1))\end{aligned}\right\} \quad (187)$$

can be written in the recursive form

$$\bar{\mathcal{G}}_k^{\beta\alpha}(t,t') = \frac{-i}{\hbar}\int_{t'}^{t} d\tau \int dy(\tau)\; G_0(\beta, y; t,\tau)\; V(y(\tau))\; \bar{\mathcal{G}}_{k-1}(y,\alpha;\tau,t') \qquad (188)$$

However this is just another way of saying that $\mathbf{G}_{\beta\alpha}$ satisfies the integral eqtn.

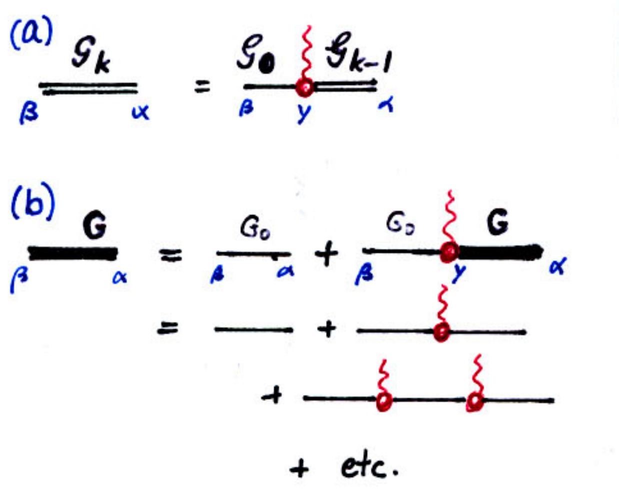
$$\boxed{\mathbf{G}^{\beta\alpha}(t,t') = G_0^{\beta\alpha}(t,t') - \frac{i}{\hbar}\int_{t'}^{t} d\tau \int dy(\tau)\; G_0(\beta, y; t,\tau)\; V(y(\tau))\; \mathbf{G}(y,\alpha;\tau,t')} \qquad (189)$$

This integral eqtn is a simple form of "Dyson's eqtn". By the usual theory of Green's functions (or of the relation between linear differential eqtns and linear integral eqtns) we can also write this in the form

$$(\mathcal{H} - i\hbar\partial_t)\,\mathbf{G}(xx'tt') = (H + V - i\hbar\partial_t)\,\mathbf{G}(xx'tt') = -i\hbar\,\delta(x-x')\,\delta(t-t') \qquad (190)$$

(cf eqtn (215) in part A). The usefullness of the integral eqtn form in (189) is precisely that it can be expanded in powers of $-iV/\hbar$, and often the expansion can then be summed.

There is of course a well-known diagrammatic representation of (188) and (189), and it is useful to get to know these representations. The way this done should be fairly clear from the diagrams shown at left.



IN (a) WE REPRESENT THE RECURSIVE EQN RELATING $\bar{\mathcal{G}}_k$ TO $\bar{\mathcal{G}}_{k-1}$ (eqtn (188)).

IN (b) WE SHOW THE DYSON EQTN (189), AND THEN IN ITS EXPANDED FORM (187). THE EXTERNAL RED VERTEX REPRESENTS THE FUNCTION $(-i/\hbar)\,V(x(\tau))$.

If we look first at (b), we see that the Green fn. $\mathbf{G}$ is represented as a thick line, whereas the bare unperturbed Green fn. G_0 is represented as a thin line. The arguments of the lines appear at each end of them. The factor associated with the perturbation, which in this case is represented by an external red line with a circle, is just

$$-\frac{i}{\hbar}\,V(y(\tau)) \qquad (191)$$

Then the rule to construct the integral eqtn is just to integrate over all internal variables in the diagram (which in this case means integrating over the variables attached to the perturbation, ie., over y and τ).

If we expand the integral eqtn in a series, by iterating, we simply re-derive the sum in (185).

The recursive eqtn in (188) is also easily represented diagrammatically, in (a) at left. With practise it becomes much easier to work with these diagrams than with the original equations, a philosophy initiated by Feynman, &

which was taken to a fine art in the "diagrammar" approach of 't Hooft & Veltman, in work on gauge theories.

These eqtns take a different form depending on which basis function one uses to represent G_0 and $\mathbf{G}$. In real space, for example, one sees that the higher-order terms in $\mathbf{G}$ involve repeated scattering of the free particle off the potential. At left we see a real spacetime path for the particle, in which it scatters 3 times off the potential $V(\underline{r})$. This is then a contribution to the 3rd-order term $\mathcal{G}_3$.

REAL-SPACE PATH CONTRIBUTING TO 3rd-ORDER DIAGRAM $\mathcal{G}_3$

Notice that $\mathcal{H}_0$ can be anything we like in this kind of theory - it is simply chosen to be solvable. In this case it is convenient to use, as a representation for the Greens fns, the eigenstates $|m\rangle$ of G_0 and $\mathcal{H}_0$, since then both of them will be diagonal. In this representation we can write

$$\mathbf{G}_{mm'}(tt') = G^0_m(tt')\,\delta_{mm'} - \tfrac{i}{\hbar}\int d\tau\, G^0_m(t,\tau')\, V_{mm''}\, G_{m''m'}(\tau,t') \qquad (192)$$

Suppose we now Fourier transform this in time, writing

$$\mathbf{G}_{mm'}(\omega) = \int dt\, e^{i\omega t}\, \mathbf{G}_{mm'}(t) = \langle m | \frac{i\hbar}{\hbar\omega - \hat{\mathcal{H}}} | m' \rangle \qquad (193)$$

(compare part A, eqtns (216) and (217)). Then Dyson's eqtn takes a particularly simple form:

$$\boxed{\mathbf{G}_{mm'}(\omega) = G^0_m(\omega)\,\delta_{mm'} + G^0_m(\omega)\, V_{mm''}\, \mathbf{G}_{m''m'}(\omega)} \qquad (194)$$

This is a matrix eqtn in the space of eigenfns of $\mathcal{H}_0$; the only thing that does not make it trivial to solve is that $V_{mm'}$ is in general non-diagonal in this basis (if it were diagonal, then the Hamiltonian $\mathcal{H}$ would also be exactly solvable). We shall have cause often to use eqtns like (194).

If we write (194) in operator form, viz

$$\hat{\mathbf{G}}(\omega) = \hat{G}_0(\omega) + \hat{G}_0(\omega)\,\hat{V}\,\hat{\mathbf{G}}(\omega) \qquad (195)$$

then we see that we can write, in symbolic form

$$\hat{\mathbf{G}}(\omega) = \left[\frac{\hat{G}_0(\omega)}{\hat{\mathbf{1}} - \hat{V}\,\hat{G}_0(\omega)}\right] \qquad (194)$$

where the operators operate in the space of eigenfunctions for the system (or some other set of complete states). Note that the right-hand side of (194) has to be seen as a single operator, ie., we can't split it into pieces except in a well-defined way like a power series.

The form (193) allows to derive a particularly simple form for the wave-functions. Recall that once we know the propagator for the system, we can also derive the wave-function $|\psi(t)\rangle$ at time t, if we know it at some other time t'. Now suppose we go over to frequency space, and imagine that we have some initial wave-function ϕ_m which is an eigenfunction of $\mathcal{H}_0$, ie., we have

$$\hat{\mathcal{H}}_0 |\psi_m\rangle \equiv \hat{\mathcal{H}}_0 |m\rangle = \epsilon_m^0 |m\rangle \qquad (195)$$

Now we rewrite (195) in the form

$$(\hat{\mathbf{1}} - \hat{V}\hat{G}_0)\,\mathbf{G} = G_0 \qquad (196)$$

and operate on $|m\rangle$. We then get

$$\left(1 - \frac{\hat{V}}{\hbar\omega - \hat{\mathcal{H}}_0}\right)|\psi\rangle = |\phi_m\rangle \qquad (197)$$

where $|\psi\rangle$ is produced by the $\mathbf{G}$ acting on $|m\rangle$: $\qquad \hat{\mathbf{G}}|\phi_m\rangle = |\psi\rangle \qquad (198)$

We rewrite (197) as

$$\boxed{|\psi\rangle = |\phi_m\rangle + \frac{\hat{V}}{\hbar\omega - \hat{\mathcal{H}}_0}|\psi\rangle} \qquad (199)$$

and we now see we have an integral eqtn for $|\psi\rangle$, the final state wave-vector, produced by adding the potential $\hat{V}$ to the original Hamiltonian $\mathcal{H}_0$. Note that we could have derived this in a much simpler way, starting from the original Schrodinger eqtn

$$(\hat{\mathcal{H}}_0 + \hat{V})|\psi\rangle = E|\psi\rangle \qquad (200)$$

If we operate on the left of (199) with the operator $(E - \hat{\mathcal{H}}_0)$, and use the identification $E = \hbar\omega$, then we immediately recover (200).

Now let's go back to our scattering problem. We shall formulate it first in a general way, and then go back to the discussion in terms of propagators.

As noted already in the last section B.1, we are concerned now with problem where the incoming state (ie., $|\phi_m\rangle$ in (199)) is a plane wave, ie., a momentum eigenstate, and $\mathcal{H}_0$ is just the free particle Hamiltonian. We write the full wave-function then in the form

$$\langle \mathbf{r}|\psi\rangle \equiv \psi(\mathbf{r}) = \begin{cases} e^{i\mathbf{k}\cdot\mathbf{r}} + \dfrac{f_k(\Theta)}{r}e^{ikr} & (3d) \\[2ex] e^{i\mathbf{k}\cdot\mathbf{r}} + \dfrac{f_k(\Theta)}{\sqrt{r}}e^{i(kr+\pi/4)} & (2d) \\[2ex] e^{ikx} + f_k^{\pm} e^{i(kx+\pi/2)} & (1d) \end{cases} \qquad (201)$$

where for simplicity we assume a centrally symmetric potential (otherwise the 3d scattering function would be a function $f_k(\theta,\phi)$ of 2 angles). The "collision" between the particle and the potential is elastic, so the scattering function is then a function only of $|\underline{k}| = k$, where $\underline{k}$ is the incoming wave-vector, and the scattering angle Θ. In the 1-d case the scattering amplitude can only depend on whether $\theta = 0, \pi$, ie., forward scattering (f^+, with $\Theta = 0$) or backward scattering (ie, f^-, or $\theta = \pi$). Since for the free particle $E = \hbar^2 k^2/2m$, we can also write $f = f(E,\theta)$.

The general theory of scattering relates $f_k(\theta)$ to both the Green function in (194) (or to its equivalent in a momentum representation, the so-called "S-matrix"), and to related functions such as the T-matrix and K-matrix. It also calculates the outgoing wave-function and complete solution $\psi(r)$, and, because we have a centrally symmetric potential, it gives useful results for all these functions in terms of phase shifts of the wave-functions. In doing all this a number of physically useful functions are defined, such as the scattering length and scattering cross-section. Finally, scattering theory provides a useful and intellectually interesting study of the analytic properties of these functions, which are complex variables depending on an energy ω which is generalized to the complex plane.

∴ Obviously scattering theory is just a special case of the development summarized in (194) and (199), with a special set of boundary conditions. These are summarized in the "Lippmann - Schwinger" eqtn, written from (199) as

$$|\psi^\pm\rangle = |\phi_{in}\rangle + \frac{\hat{V}}{E - \hat{\mathcal{H}}_0 \pm i\delta}|\psi^\pm\rangle \tag{202}$$

or in real space representation, for d dimensions,

$$\langle \underline{r}|\psi^\pm\rangle = \langle r|\phi_{in}\rangle + \int d^d r' \, G_0^\pm(\underline{r}-\underline{r}') \langle \underline{r}'|V|\psi^\pm\rangle \tag{203}$$

where the "±" signify the particular boundary conditions appropriate to "retarded" (outgoing) or "advanced" (ingoing) scattered waves; the momentum space form of (203) is

$$\psi_{\underline{k}}^\pm = \phi_{\underline{k}}^{in} + G_0^\pm(\underline{k}) \sum_{k'} V_{\underline{k}\underline{k}'} \psi^\pm_{\underline{k}'} \tag{204}$$

We can see that the form chosen for $\hat{G}_0^\pm$ does enforce the correct boundary conditions in several ways. One is simply to calculate the real space form for $G_0^\pm(\underline{r},\underline{r}')$; it is given by

$$G_0^\pm(\underline{r},\underline{r}';E) \equiv \langle \underline{r}|\frac{1}{E - \hat{\mathcal{H}}_0 \pm i\delta}|\underline{r}'\rangle = \sum_{k'} \frac{e^{i\underline{k}'(\underline{r}-\underline{r}')}}{E - \hbar^2 k'^2/2m \pm i\delta} \tag{205}$$

This Fourier transform can be done in 1-d, 2-d or 3-d; let's do it for 3d, where we get

(3d)

$$\left.\begin{aligned} G_0^\pm(r,r';E) &= \frac{2m}{\hbar^2}\int \frac{d^3k'}{(2\pi)^3} \frac{e^{ik'\cdot(r-r')}}{k^2 - k'^2 \pm i\delta} \\ &= \frac{m}{4\pi^3\hbar^2}\int_0^{2\pi} d\phi \int_{-1}^{1} d\mu \int_0^\infty k'^2 dk' \frac{e^{ik'\mu|\underline{r}-\underline{r}'|}}{k^2 - k'^2 \pm i\delta} \\ &= \frac{i m}{4\pi^2\hbar^2}\frac{1}{|\underline{r}-\underline{r}'|}\int_{-\infty}^{\infty} dk' \, e^{ik'|r-r'|}\left[\frac{1}{k' - (k \pm i\delta)} + \frac{1}{k' + (k \pm i\delta)}\right] \\ &= -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{\mp ik|r-r'|}}{|r-r'|} \end{aligned}\right\} \tag{206}$$

from which we see the required result, viz., that $G_0^{\pm}(r,r';E)$ represents a wave either being scattered out from $\underline{r}'$ to $\underline{r}$, or scattered in from $\underline{r}$ to $\underline{r}'$.

Another way to see the same result is to go over to a time-dependent picture, and imagine switching on the potential $V(\underline{r})$ to its value at time t from zero at time $t \to \pm\infty$, using the device of a multiplier $e^{\pm\delta t}$ - this gives the same result.

We now observe that we have actually derived the form in (201) for the 3d scattering solution, provided we take $k_0(r-r') \gg 1$, and assume that $|r-r'| \gg \ell_0$ where ℓ_0 is the range of the scattering potential (we will define this more precisely later on). Then we can write

$$e^{\pm i\underline{k}'\cdot(r-r')} \sim e^{\pm ik'r}\, e^{\mp i\underline{k}'\cdot r'} \qquad (r \gg \ell_0) \qquad (207)$$

and in the 3d case we have, from (203), and using $\langle r|\phi_m\rangle = \langle \underline{r}|\underline{k}\rangle$ (208)

the result that

$$\langle \underline{r}|\psi_k^+\rangle \xrightarrow[r \gg \ell_0]{} \langle r|\underline{k}\rangle + \frac{f(\underline{k}',\underline{k})}{r}e^{ikr} \qquad (3d) \qquad (210)$$

where

$$f(k',k) = -\frac{2m}{\hbar^2}\pi^2\langle k'|V|\psi_k^+\rangle \qquad (3d) \qquad (211)$$

Quite generally, we see that in d dimensions:

$$\frac{f(k',k)}{r^{d/2-1}} \equiv \frac{f_k(\theta)}{r^{d/2-1}} = e^{-ikr}\int d^d r'\, G_0^+(\underline{r}-\underline{r}')\langle \underline{r}'|V|\psi_k^+\rangle \qquad (212)$$

Now eqtns like (194), (199), and (203) are integral eqtns in which the solution appears on both sides of the equation. It is given formally by iteration of these eqtns to infinite order - from any of these forms we can see that our dimensionless expansion parameter is the operator

$$\hat{\lambda}(z) = \hat{V}G_0(z) = \frac{\hat{V}}{z-\hat{\mathcal{H}}_0} \qquad (213)$$

and we see that the formal expansion is of course just the diagrammatic expansion:

$$\hat{G}(z) = \hat{G}_0(z)\sum_{n=0}^{\infty}\hat{\lambda}^n(z) \qquad (214)$$

The study of such integral eqtns was carried out by Schmidt, Fredholm, Neumann, & Volterra in the early-mid 19th century, and has been employed in great detail in modern scattering theory. Here we will just touch on it, in the next section. Notice that the lowest order term in the expansion gives the "Born approximation" for the scattering amplitude - one has

$$\frac{f_k(\theta)}{r^{d/2-1}}e^{ikr} \xrightarrow[\text{Born}]{} \frac{\hat{V}}{E-\hat{\mathcal{H}}_0+i\delta}|\phi_k^{in}\rangle = \int d^d r'\, G_0^+(\underline{r}-\underline{r}')\langle \underline{r}'|V|k\rangle \qquad (215)$$

where in the integral eqtn we simply substitute $|\psi_k^\pm\rangle \to |\phi_k^\pm\rangle$ on the right-hand side. This is easily worked out since $|\phi_k\rangle$ is just a plane wave. Thus, eg., in 3d we have

$$f_k^{Born}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\langle \underline{k}'|V|\underline{k}\rangle = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\, e^{i(k-k')r'} V(r') \quad (3d) \qquad (216)$$

which for a centrally symmetric potential gives

$$f_k^{Born}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{|k-k'|}\int_0^\infty r\,dr\, V(r)\sin(|k-k'|r) \quad (3d) \qquad (217)$$

One can work out similar results in 1d and 2d

B.2.1. (b) SCATTERING FUNCTIONS

: It is useful to define a set of functions which are related to the scattering function $f_{kk'}$ and the propagator $G_{kk'}(\omega)$, and generalize them to the complex energy plane. We begin with the "S-matrix", defined between initial & final states as

$$\hat{S}_{fi} = \lim_{t\to\infty}\lim_{t'\to-\infty}\langle\psi_f(t)|\hat{G}(t,t')|\psi_i(t')\rangle \qquad (218)$$

where $G_{kk'}(tt')$ is the Green function we already defined, in which the initial state is a plane wave coming into the scattering potential, and the final state a plane wave leaving it.

We then define the T-matrix, initially by the equation

$$\hat{V}|\Psi_k^+\rangle = \hat{T}|\phi_k\rangle \qquad (219)$$

ie, the operator $\hat{T}$ acting on the initial state is equivalent to the operation of $\hat{V}$ on the full solution $|\Psi_k^+\rangle$. Consider now the Lippmann-Schwinger eqtn, in the form (202); if we multiply it on the left by $\hat{V}$, we get, using (219), that

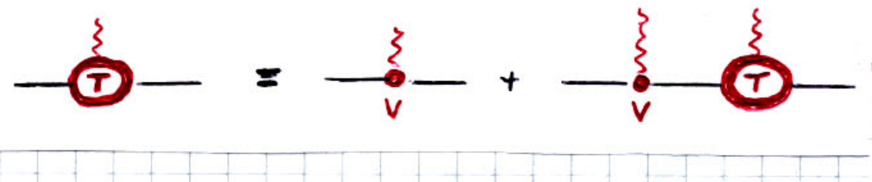
$$\hat{T}|\phi_k\rangle = \left[\hat{V} + \hat{V}\frac{1}{E-\hat{H}_0+i\delta}\hat{T}\right]|\phi_k\rangle \qquad (220)$$

or, multiplying on the left again with $\langle\phi_{k'}|$, we get

$$T_{k'k} = V_{k'k} + V_{k'k''}G_0^+(k'')T_{k''k} \qquad (221)$$

If we now continue the energy $E = \hbar\omega$ to the complex plane, we have the general relation

$$\boxed{\hat{T}(z) = \hat{V} + \frac{\hat{V}}{z-\hat{H}_0}\hat{T}(z) \equiv \hat{V} + \hat{V}G_0(z)\hat{T}(z)} \qquad (222)$$



This result is more or less obvious diagrammatically, if we iterate the expansion at left or in (222), and compare with the iterated expansion for $G(z)$, which is given by continuing (195) to the complex energy plane:

$$\left.\begin{aligned}\hat{G}(z) &= \hat{G}_0(z) + \hat{G}_0(z)\hat{V}G(z) \\ &= \hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)\end{aligned}\right\} \tag{223}$$

whose 2nd form is obvious from the diagrams, or by operating "on" (222) on the left with V^{-1}, and on the right with $G_0(z)$.

Another operator related to this one is the "K-matrix", or reactance matrix, which is defined only on the energy shell (ie, for $z \to$ real ω):

$$\hat{K}(\epsilon) = \hat{V} + \hat{V}\hat{\mathbb{P}}\frac{1}{E - \hat{H}_0}K(E) \tag{224}$$

where $\hat{\mathbb{P}}$ refers to the principal part; This is defined for the operation of integration by

$$\int_{-\infty}^{\infty} dE\, \hat{\mathbb{P}}\frac{1}{E-x}f(\epsilon) \equiv \lim_{\epsilon \to 0}\int_{-\infty}^{x-\epsilon} dE + \int_{x+\epsilon}^{\infty} dE\left(\frac{f(\epsilon)}{E-x}\right) \tag{225}$$

Now consider the relation between these functions. We have $\boxed{|\Psi^+\rangle = \hat{S}|\phi_k\rangle}$ (226)

by definition of $\hat{S}$; and also that $\boxed{|S|^2 = 1}$ (227)

which follows because $\hat{S}$ & $\hat{G}$ are unitary.

Now suppose we compare the time-retarded and advanced solutions to the Lippmann-Schwinger eqtn; note that we can write, in analogy to (199) or (202), that

$$\langle\Psi^-| = \langle\phi_k| + \langle\Psi^-|\frac{V}{E - \hat{H}_0 - i\delta} \tag{228}$$

Then the vector product $\langle\phi_{k'}|\Psi_k^+\rangle$ (with ingoing/outgoing waves having momentum k', k, respectively),

$$\left.\begin{aligned}\langle\phi_{k'}|\psi_k^+\rangle &= \langle\phi_{k'}|\phi_k\rangle + \left[\frac{1}{E-\hat{H}_0+i\delta} - \frac{1}{E-\hat{H}_0-i\delta}\right]\langle\phi_{k'}|V|\psi_k^+\rangle \\ &= \delta_{kk'} - 2\pi i\,\delta(E-\hat{H}_0)\langle\phi_{k'}|V|\psi_k^+\rangle\end{aligned}\right\} \tag{229}$$

which is the same as saying that $\boxed{\hat{S}(E) = 1 - 2\pi i\,\delta(E-\hat{H}_0)\,\hat{T}(E)}$ (230)

In the same way we can show $\boxed{\frac{1-\hat{S}(E)}{1+\hat{S}(E)} = 2\pi\,\delta(E-\hat{H}_0)\,K(E)}$ (231)

Now we would like to relate these quantities to the scattering function $f_{kk'}$. However the details of this depend on how many dimensions we are working in, so we will do this for different dimensions in turn.

Before doing this it is useful to discuss the way in which one can expand all these functions in the appropriate eigenfunctions of the Hamiltonian operator. This is crucial when one wants to do practical calculations

PARTIAL WAVE EXPANSIONS : To expand the various functions in terms of these eigenfunctions, we first need to know what they are. We also wish to know the form of the Green functions for the wave equation. The results are as follows:

3 dimensions : If we deal with a centrally symmetric potential, then we can expand in terms of the complete set of eigenfunctions of the free-particle Schrodinger eqtn; ie. we can write expansion of the form (for central potentials):

$$\Psi(r,\theta,\phi) = \sum_{lm} c_{lm} R_l(r) Y_{lm}(\theta,\phi) \tag{232}$$

where

$$Y_{lm}(\theta,\phi) = (-1)^m \left(\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right)^{1/2} e^{im\phi} P_l^m(\theta) \tag{233}$$

where

$$P_l^m(\theta) = \frac{(-1)^{m+l}}{2^l l!}\frac{(l+|m|)!}{(l-|m|)!} \sin^{-|m|}\theta \left(\frac{d}{d\cos\theta}\right)^{l-|m|} \sin^{2l}\theta \tag{234}$$

is the associated Legendre polynomial; and the radial function can be expanded as

$$R_l(r) = a_l j_l(r) + b_l n_l(r) \tag{235}$$

where

$$\left.\begin{aligned} j_l(r) &= \left(\frac{\pi}{2r}\right)^{1/2} J_{l+1/2}(r) \\ n_l(r) &= \left(\frac{\pi}{2r}\right)^{1/2} Y_{l+1/2}(r) \end{aligned}\right\} \tag{236}$$

are spherical Bessel functions. The properties of all these functions, and their use in 3-d scattering problems, are discussed in any good book on Q.M. We have already calculated the Green function for the 3-d free particle (see (206)): we reiterate the result here

$$\left.\begin{aligned} G_0^{\pm}(k;E) &= \frac{1}{E - \hbar^2k^2/2m \pm i\delta} \\ G_0^{\pm}(r,r';E) &= \sum_{k'} e^{ik'\cdot(r-r')} G_{k'}(E) \\ &= -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{\mp ik|r-r'|}}{|r-r'|} \end{aligned}\right\} (3d) \tag{238}$$

To analyse the scattering problem we need to know how to expand both the plane wave form $e^{ik\cdot r}$ and the scattered wave, in the ansatz (201), in terms of these functions. Let us choose the incoming wave to be along the $\hat{z}$-direction, so $e^{ik\cdot r} \to e^{ikz}$.

Then we can do the expansion - it turns out to be

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(kr) P_l(\cos\theta) \qquad (3d) \qquad (239)$$

which is a special case of

$$e^{i\underline{k}\cdot\underline{r}} = 4\pi \sum_{lm} i^l j_l(kr)\, Y^*_{lm}(\hat{\underline{k}})\, Y_{lm}(\hat{\underline{r}}) \qquad (3d) \qquad (240)$$

obtained by applying the addition theorem

$$P_l(\hat{\underline{k}}\cdot\hat{\underline{k}}') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\underline{k})\, Y^*_{lm}(\underline{k}') \qquad (3d) \qquad (241)$$

where $\hat{k}, \hat{k}'$ are unit vectors, and $\underline{k}\cdot\underline{k}' = \cos\theta_{kk'}$. The asymptotic behaviour of the function e^{ikz} is just

$$e^{ikz} \xrightarrow[kr \gg 1]{} \frac{1}{kr} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) \sin(kr - \pi l/2) \qquad (242)$$

Now let us compare the asymptotic behaviour here with that of the assumed solution in (232) and (235), which must have the form

$$\Psi^+(r,\theta) \xrightarrow[kr \gg 1]{} \sum_l A_l (2l+1)\, i^l P_l(\cos\theta) \frac{1}{kr} \sin(kr - \tfrac{\pi l}{2} + \delta_l) \qquad (3d) \qquad (243)$$

where we ignore any dependence on the azimuthal angle since the problem is cylindrically symmetric. If we now compare with (201), we see that

$$\frac{f_k(\theta)}{r} e^{ikr} = \Psi(r,\theta) - e^{ikz} \qquad (244)$$

which fixes $A_l = e^{i\delta_l}$, and gives the result

$$f_k(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l(k)} - 1) P_l(\cos\theta) \qquad (245)$$

which we write as

$$f_k(\theta) = \sum_l (2l+1) f_l(k) P_l(\cos\theta) \qquad (246)$$

where

$$\boxed{\begin{aligned} f_l &= \frac{1}{2ik}(S_l(k) - 1) \\ S_l(k) &= e^{2i\delta_l(k)} \end{aligned}} \qquad (247)$$

To see what this means, note that the original incoming plane wave solution can be written as

$$e^{ikz} \underset{kr \gg 1}{\sim} \sum_{l=0}^{\infty} \frac{1}{2ikr} (2l+1) P_l(\cos\theta) \left[e^{ikr} - e^{-i(kr - \pi l)} \right] \qquad (248)$$

whereas the final solution

$$\Psi^+(r,\theta) \underset{kr \gg 1}{\sim} \sum_{l=0}^{\infty} \frac{1}{2ikr} (2l+1) P_l(\cos\theta) \left[S_l(k) e^{ikr} - e^{-i(kr - \pi l)} \right] \qquad (249)$$

Thus we see that the incoming plane wave is a simple superposition of retarded and advanced waves, phase-shifted by $\ell\pi/2$ in the ℓ-th angular component; and that the only effect of the scatterer is to multiply the outgoing wave (retarded wave) by the unitary operator S_ℓ (in the ℓ-th angular channel).

From this we see that S_ℓ is just the ℓ-th angular component of the S-matrix - we make this precise below. All that S_ℓ does is "rotate" the wave function in Hilbert space (the outgoing part).

It is useful to write a few other identities for the $f_\ell(k)$. We have

$$f_\ell(k) = \frac{1}{k} e^{i\delta_\ell(k)} \sin\delta_\ell(k) \tag{250}$$

so

$$\mathrm{Im}\, f_\ell(k) = \frac{1}{k}\sin^2\delta_\ell(k) = k\,|f_\ell(k)|^2 \tag{251}$$

Moreover

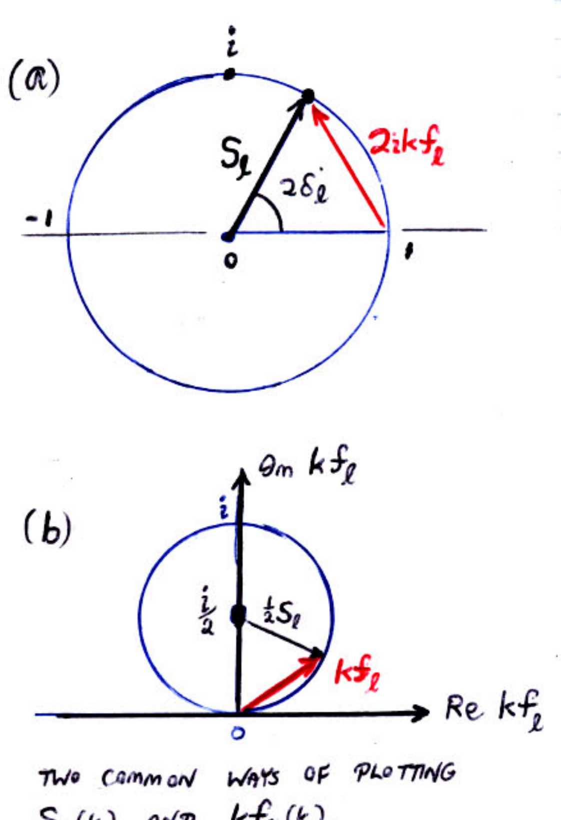
$$\mathrm{Im}\left(1/f_\ell(k)\right) = -k \tag{252}$$

so one can usefully write

$$\left.\begin{aligned} f_\ell(k) &= \frac{1}{g_\ell(k) - ik} \\ g_\ell(k) &= k\cot\delta_\ell(k) \end{aligned}\right\} \tag{253}$$

where $g_\ell(k)$ is real. We also notice that (251) is just:

$$2i\,\mathrm{Im}\, f_\ell(k) = \left(f_\ell(k) - f_\ell^*(k)\right) = 2ik\, f_\ell(k) f_\ell^*(k) \tag{254}$$



TWO COMMON WAYS OF PLOTTING $S_\ell(k)$ AND $kf_\ell(k)$.

These relations make it convenient to plot the functions

$$S_\ell(k) = 1 + 2ik\, f_\ell(k) \tag{255}$$

and $f_\ell(k)$ in an Argand diagram - the 2 most useful ones are shown at left. In the first we simply plot $S_\ell(k)$, which is a unit vector at an angle $2\delta_\ell(k)$ from the real axis - see plot (a) at left.

In the 2nd plot (b) at left we show the function $kf_\ell(k)$.

One can also define the real function

$$\left.\begin{aligned} K_\ell(k) &= -\tan\delta_\ell(k) \\ &= -k/g_\ell(k) \end{aligned}\right\} \tag{256}$$

We notice that $K_\ell(k)$ is singular whenever $\delta_\ell(k)$ passes through a phase $(2n+1)\pi/2$, and we shall see later the significance of this result. The functions $K_\ell(k)$, and the operator $K(E)$ in (231), are sometimes referred to as the "Reaction matrix", or the "Reaction operator".

2 dimensions : The partial wave expansion is a little simpler in 2d, but it has the same basic structure as the 3d expansion. We have already seen this kind of expansion in section (pp 104-110). We can write the solution to Schrodinger's eqtn in the form

$$\Psi(r,\theta) = \sum R_\ell(r)\,\chi_\ell(\theta) \tag{257}$$

where
$$\chi_\ell(\theta) = \frac{1}{\sqrt{2\pi}}\,e^{i\ell\theta} \tag{258}$$

and we expand $R_\ell(r)$ in the form

$$R_\ell(r) = a_\ell J_\ell(kr) + b_\ell Y_\ell(kr) \tag{259}$$

The 2-d Green function for this problem is more difficult to get than the 3d form; we have

$$\left.\begin{aligned} G_0^+(r,r';E) &= \frac{2m}{\hbar^2}\int\frac{d^2k'}{(2\pi)^2}\,\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{k^2-(k')^2+i\delta} \\ &= \frac{2m}{\hbar^2}\int_0^{2\pi}\frac{d\theta}{2\pi}\int\frac{k'dk'}{2\pi}\,\frac{e^{ik'|\mathbf{r}-\mathbf{r}'|\cos\theta}}{k^2-(k')^2+i\delta}\end{aligned}\right\} \tag{260}$$

and then, if we do the θ-integral first, using: $\displaystyle\int_0^{2\pi}\frac{d\theta}{2\pi}e^{i\alpha\cos\theta} = J_0(\alpha)$ (261)

and then using the identity:
$$\left.\begin{aligned}\int\frac{x\,dx}{x^2-k^2}J_\nu(ax)J_\nu(bx) &= \frac{i\pi}{2}J_\nu(ak)H_\nu^+(bk) \\ (b>a\ ;\ \mathrm{Re}\,\nu &> -1)\end{aligned}\right\} \tag{262}$$

we get, taking $a\to 0$, that

$$\left.\begin{aligned} G_0^+(r,r';E) &= \frac{-im}{2\hbar^2}\,H_0^+(k|\mathbf{r}-\mathbf{r}'|) \\ G_0^+(k,E) &= \frac{1}{E-\hbar^2k^2/2m+i\delta}\end{aligned}\right\}\ (2d) \tag{263}$$

which, incidentally, has the following asymptotic properties:

$$\left.\begin{aligned} G_0^+(r,E) &\xrightarrow{kr\gg 1} \frac{-im}{2\hbar^2}\left(\frac{2}{\pi kr}\right)^{1/2}e^{i(kr-\pi/4)} \\ &\xrightarrow{kr\ll 1} \frac{m}{\pi\hbar^2}\left[\ln\left(\frac{C_1 kr}{2}\right)-i\frac{\pi}{2}\right]\end{aligned}\right\}\ (2d) \tag{264}$$

If we now assume an incoming wave $e^{ikx} = e^{ikr\cos\theta}$, then we can resolve this as

$$\left.\begin{aligned} e^{ikx} &= \sum_{\ell=-\infty}^{\infty} i^\ell J_\ell(kr)\,e^{i\ell\theta} \\ &\xrightarrow{kr\gg 1} \left(\frac{2}{\pi kr}\right)^{1/2}\sum_\ell i^\ell e^{i\ell\theta}\cos\left(kr-\frac{\pi}{2}(\ell+1/2)\right)\end{aligned}\right\} \tag{265}$$

We now go through the familiar routine, familiar from the 3d method and from our work on 2d scattering problems before, and assume a solution for the outgoing wave-function of the form in (259), which has the asymptotic form

$$\Psi(r,\theta) \xrightarrow[kr \gg 1]{} \left(\frac{2}{\pi kr}\right)^{1/2} \sum_\ell A_\ell i^\ell e^{i\ell\theta} \cos\left(kr - \tfrac{\pi}{2}(\ell + \tfrac{1}{2}) + \delta_\ell\right) \qquad (266)$$

and again we find, by matching solutions, that $A_\ell = e^{i\delta_\ell}$, and that now

$$f_k(\theta) = \left\{ \begin{array}{l} -i\left(\frac{1}{2\pi k}\right)^{1/2} \sum_\ell \left(e^{2i\delta_\ell(k)} - 1\right) e^{i\ell\theta} \\ \left(\frac{2}{\pi k}\right)^{1/2} \sum_\ell e^{i\delta_\ell(k)} \sin\delta_\ell(k)\, e^{i\ell\theta} \end{array} \right\} = \sum_\ell f_\ell(k) e^{i\ell\theta} \qquad (267)$$

so that
$$S_\ell(k) = 1 + 2i\left(\frac{\pi k}{2}\right)^{1/2} f_\ell(k) \qquad (268)$$

and
$$f_\ell(k) = \left(\frac{2}{\pi k}\right)^{1/2} e^{i\delta_\ell(k)} \sin\delta_\ell(k) = \left(\frac{2}{\pi k}\right)^{1/2} \frac{1}{\cot\delta_\ell(k) - i} \qquad (269)$$

<u>1 dimension</u>: This case is rather trivial, but we give the results all the same. All solutions and scattering functions depend only on waves moving either forward or backwards. One has scattering solution of form

$$\psi(x) = \sum_\pm a_\pm e^{\pm ikx} \qquad (270)$$

and the Green function is found to be

$$\left. \begin{aligned} G_0^+(x-x'; E) &= \sum_{k'} e^{ik'(x-x')} G^0_{k'}(E) \\ &= \frac{-im}{\hbar^2 k} e^{ik|x-x'|} \end{aligned} \right\} \qquad (271)$$

Now, when we compare scattered waves and incoming waves, we simply compare e^{ikx} with a scattered wave $e^{i(kx+\delta)}$. We then write:

$$S_k = 1 + 2if_k = \frac{k - ig_k}{k + ig_k} = e^{2i\delta_k} \qquad (272)$$

so that
$$f_k = \frac{ig_k}{g_k - ik} = e^{i\delta_k} \sin\delta_k = \frac{1}{\cot\delta_k - i} \qquad (273)$$

$$g_k = -k \tan\delta_k \qquad (274)$$

NB: compare pp 93-96, where we studied a δ-fn potential. For that case, we see that $g_k \to g_0$ for a potential barrier, ie.

If
$$V(x) = V_0\delta(x) = \frac{\hbar^2}{m} g_0 \Rightarrow g_k \to g_0 \qquad (275)$$

and
$$\delta_k \to -\tan^{-1}(g_0/k) \qquad (276)$$

SCATTERING CROSS-SECTION : In any real experiment in particle physics, one is interested in the total scattering probability. Since $f_k(\theta)$ is the amplitude of the outgoing wave, it then follows that

$$\sigma_k^{Tot} = \begin{cases} \int d\Omega_\theta \, \sigma_k(\theta) & (3d) \\ \int d\theta \, \sigma_k(\theta) & (2d) \end{cases} \tag{277}$$

where $\sigma_k(\theta)$ (sometimes called the "differential scattering cross-section", and written as $d\sigma/d\Omega$ or $d\sigma/d\theta$) is just

$$\sigma_k(\theta) = |f_k(\theta)|^2 \tag{278}$$

If we write:
$$\sigma_k^{Tot} = \sum_\ell \sigma_\ell(k) \tag{279}$$

Then we have

$$\sigma_\ell(k) = \left\{ \begin{array}{ll} 4\pi(2\ell+1)\,|f_\ell(k)|^2 & (3d) \\ 2\pi\,|f_\ell(k)|^2 & (2d) \\ |f_k|^2 & (1d) \end{array} \right\} \tag{280}$$

where

$$\left. \begin{array}{lll} |f_\ell(k)|^2 = \frac{1}{k^2}\sin^2\delta_\ell(k) & & (3d) \\ |f_\ell(k)|^2 = \frac{2}{\pi k}\sin^2\delta_\ell(k) & & (2d) \\ |f_k|^2 = \sin^2\delta_k & & (1d) \end{array} \right\} \tag{281}$$

Notice that for 1-d systems we can rewrite this as

$$|f_k|^2 = \frac{g_k^2}{k^2 + g_k^2} \quad (1d) \tag{282}$$

Thus we summarize these results for the total cross-section:

$$\sigma_k^{Tot} = \left\{ \begin{array}{ll} 4\pi/k^2 \sum_\ell (2\ell+1)\sin^2\delta_\ell(k) & (3d) \\ \frac{4}{k}\sum_\ell \sin^2\delta_\ell(k) & (2d) \\ \sin^2\delta_k & (1d) \end{array} \right\} \tag{283}$$

Now consider the quantity $\mathrm{Im}\, f_k(\theta)$, for $\theta \to 0$; this is the imaginary part of the forward scattering amplitude. We have

$$\mathrm{Im}\, f_k(\theta\to 0) = \left\{ \begin{array}{ll} 1/k \sum_\ell (2\ell+1)\sin^2\delta_\ell(k) & (3d) \\ (2/\pi k)^{1/2} \sum_\ell \sin^2\delta_\ell(k) & (2d) \\ \sin^2\delta_k & (1d) \end{array} \right\} \tag{284}$$

from which we see that

$$\sigma_k^{Tot} / \Im m\, f_k(\theta \to 0) = \left\{ \begin{array}{ll} \frac{4\pi}{k} & (3d) \\ (8\pi/k)^{1/2} & (2d) \\ 1 & (1d) \end{array} \right\} \qquad (285)$$

This result, that σ_k^{Tot} is proportional to $\Im m\, f_k(\theta \to 0)$ is known as the OPTICAL THEOREM. We see that since σ_k^{Tot} is proportional to a sum over $|f_\ell|^2$, and so is $\Im m\, f_k(\theta)$, then the real reason for the result is that

$$\Im m\, f_\ell(k) \propto |f_\ell(k)|^2 \qquad (286)$$

in any dimension - in fact we have

$$\Im m\, f_\ell(k) / |f_\ell(k)|^2 = \alpha_k = \left\{ \begin{array}{ll} k & (3d) \\ (\pi k/2)^{1/2} & (2d) \\ 1 & (1d) \end{array} \right\} \qquad (287)$$

where we write $$S_\ell(k) = e^{2i\delta_\ell(k)} = 1 + 2i\alpha_k f_\ell(k) \qquad (288)$$

for any dimension. Since $|S_\ell(k)| = 1$ because of the conservation of probability, it is clear that the optical theorem also has to do with this same conservation law - we will prove this later on.

Finally, we note the idea of the "scattering length". Let us consider the very long wavelength limit for scattering, when $k \to 0$. Then it is clear that in 2d & in 3d, only the $\ell = 0$ channel will contribute to the scattering - this is obvious both physically and from the form of the radial eqtn.

So now consider the scattering cross section in this limit. - we can write it as

$$\sigma_k^{Tot} \xrightarrow{k\to 0} \sigma_{\ell=0}(k) = \Omega_d |f_0(k)|^2 \qquad (289)$$

where Ω_d is the "solid angle" for a hypersphere in d dimensions, ie $\Omega_d = 4\pi$ in 3d, $\Omega_d = 2\pi$ in 2d, and $\Omega_d = 1$ in 1d.

It is the conventional to define the "SCATTERING LENGTH" in 3d problems, so that $\sigma_k^{Tot} \xrightarrow[k\to 0]{} 4\pi a_0^2$. Here we shall generalize this and write

$$\left. \begin{array}{l} \sigma_k^{Tot} \xrightarrow[k\to 0]{} \Omega_d\, a_0^2 \\ a_0 = |f_0(k)|_{k\to 0} = \frac{1}{\alpha_k} \sin \delta_0(0) \end{array} \right\} \qquad (290)$$

Note that only in 3 dimensions is a_0 actually a length!

RELATIONS between SCATTERING FUNCTIONS

: To complete the formal apparatus for calculating scattering amplitudes, phase shifts, cross-sections, etc., we need to determine the connections between functions like $\hat{S}$, $\hat{T}$, which are operators defined in terms of the propagator $\hat{G}$ and the potential $\hat{V}$, and the functions like $f_{kk'}$, $\delta_\ell(k)$, etc., which are defined by the ansatz in (201).

Here I give a list of these relations. There is no general agreement in the literature about how these should be written, for 2 reasons, viz.

(i) Many authors do not include the factor $(2m/\hbar^2)$ which appears when one converts integrals to dimensionless form (compare, eg., eqtns (14) or (238) in this section B)

(ii) In any Fourier transform there are factors of $(2\pi)^d$ (where d is the space dimension) floating around, and it is a matter of convention where one puts these.

With this in mind, we can give the relationships between the various quantities in one specific convention. We can do this by starting from the definition of the T-matrix in (219), which we write as:

$$T_{\underline{k}\underline{k}'} \equiv \langle \phi_{\underline{k}} | \hat{T} | \phi_{\underline{k}'} \rangle = \langle \phi_{\underline{k}} | \hat{V} | \Psi^+_{\underline{k}'} \rangle = \langle \underline{k} | \underline{r} \rangle \langle \underline{r} | \hat{V} \Psi^+ | \underline{r} \rangle \langle \underline{r} | \underline{k}' \rangle \qquad (291)$$

ie.,

$$T_{kk'} = \int d^d r \, e^{i(\underline{k}-\underline{k}')\cdot\underline{r}} \, V(r) \, \Psi^+(\underline{r}) \qquad (292)$$

and then use our expressions for $\Psi^+(r)$ which we have obtained in terms of the f-function $f_{kk'}$. Alternatively, we can start from the defining equation for the S-matrix in terms of the T-matrix (eqtn. (230)), and compare it with the expressions (288) and (287) which relate the angular components of S to those of the f-function. The latter way is quicker. Let us define

$$\left.\begin{array}{lll} T_k(\theta) & = \left\{ \begin{array}{l} \sum_\ell (2\ell+1)\, t_\ell(k)\, P_\ell(\cos\theta) \\ \sum_\ell t_\ell(k) \cos(\ell\theta) \end{array} \right. & \begin{array}{l} (3d) \\ (2d) \end{array} \\ T_k & = t_k & (1d) \end{array}\right\} \qquad (293)$$

in analogy with our definition of the $f_\ell(k)$. It then follows, by comparing (230) with (287) and (288), that

$$\pi\delta(E-\hat{H}_0)\, t_\ell(k) = -\alpha_\ell f_\ell(k) = \left\{ \begin{array}{ll} -k f_\ell(k) & (3d) \\ -(\pi k/2)^{1/2} f_\ell(k) & (2d) \\ -f_\ell & (1d) \end{array} \right\} \qquad (294)$$

How we write the relationship between $T_{kk'}$ and $f_{kk'}$ depends on how we handle the $\delta(E-\hat{H}_0)$ term when we go to momentum space, how we include the $(2\pi)^d$ terms, and whether we include the factor $2m/\hbar^2$.

In what follows we will do it one way, and use that convention from here on. A warning - the literature is very confusing!

What we will do is calculate the relationship between the f-function and the matrix elements $T_{kk'}$ of the T-matrix, computed on the energy shell. The results are initially confusing because this T-matrix is not the same as the function $\hat{T}(E)\,\delta(E-H_0)$ which we have already discussed.

Relation between $f_{kk'}$ and $T_{kk'}$: Let's compute this for the cases of 1, 2, and 3 dimensions. The technique is the same in all 3 cases:

1 dimension : We want to compare the expression for the scattered wave calculated using the scattering equation, with that for the same scattered wave in terms of the f-function. First, the T-matrix equation:

$$\left.\begin{aligned} \psi^+(x) &= e^{ikx} + \int dx'\, G_0^+(x-x')\,\langle x'|V|\psi^+\rangle \\ &= e^{ikx} + \psi^+_{scatt}(x) \end{aligned}\right\} \quad (1d) \qquad (295)$$

where the scattered wave is, using (291), given by

$$\left.\begin{aligned} \psi_{scatt}(x) &= \frac{2m}{\hbar^2}\frac{-i}{2k}\, e^{ikx}\int dx'\, e^{-ik'x'}\,V(x')\,\psi^+(x') \\ &= \frac{2m}{\hbar^2}\frac{-i}{2k}\, e^{ikx}\,\langle k'|V|\psi^+\rangle \\ &= \frac{2m}{\hbar^2}\frac{-i}{2k}\, T_{kk'}\, e^{ikx} \end{aligned}\right\} \quad (1d) \qquad (296)$$

This is to be compared with the scattered wave described by the f-function, which from (201) is

$$\psi_{scatt}(x) = f_{kk'}\, e^{i(kx+\pi/2)} \qquad (1d) \qquad (297)$$

and so we get

$$f_{kk'} = \frac{-2m}{\hbar^2}\frac{1}{2k}\, T_{kk'} \qquad (1d) \qquad (298)$$

Note that we can compare this with the result in (273), ie., we write $q = k-k'$, and

$$f_{kk'} = \frac{i g_q}{g_q - iq} = \frac{-g_q}{q}\frac{1}{1+ig_q/q} = -\frac{g_q}{q}\sum_{n=0}^{\infty}\left(\frac{-ig_q}{q}\right)^n \qquad (1d) \qquad (299)$$

so that

$$T_{kk'} = \frac{\hbar^2}{m}\, g_q\, \frac{1}{1+i\,g_q/q} \qquad (1d) \qquad (300)$$

For the δ-fn potential $V_0\,\delta(x) = \frac{\hbar^2}{m}\, g_0\,\delta(x)$, so that $g_q = g_0$, we have

$$T_{kk'} \longrightarrow V_0\,\frac{1}{1+i\,\frac{m}{\hbar^2}V_0/q} \qquad (V_{kk'} \to V_0) \qquad (301)$$

2 dimensions: We now have

$$\psi^+(\underline{r}) = e^{ikx} + \int d^2r'\, G_0^+(\underline{r}-\underline{r}')\, \langle \underline{r}'|V|\psi^+\rangle \qquad (2d) \qquad (302)$$

so that, using (263) and (264), we have

$$\psi_{scatt}(\underline{r}) = \frac{2m}{\hbar^2}\frac{-i}{4}\int d^2r'\, H_0^+(k|\underline{r}-\underline{r}'|)\, V(\underline{r}')\psi^+(\underline{r}') \qquad (2d) \qquad (303)$$

$$\left.\begin{aligned} &\xrightarrow[kr \gg 1]{} -\frac{2m}{\hbar^2}\frac{1}{2}\left(\frac{1}{2\pi k}\right)^{1/2}\frac{e^{i(kr+\pi/4)}}{\sqrt{r}}\int d^2r'\, e^{-ik'r'}\, V(r')\psi^+(r') \\ &= \frac{2m}{\hbar^2}\frac{-1}{2}\frac{1}{(2\pi k)^{1/2}}\, T_{kk'}\, \frac{e^{i(kr+\pi/4)}}{\sqrt{r}} \end{aligned}\right\} \qquad (304)$$

so that, comparing with (201), we get

$$f_{kk'} = -\frac{2m}{\hbar^2}\frac{1}{2(2\pi k)^{1/2}}\, T_{kk'} \qquad (2d) \qquad (305)$$

3 dimensions: We now have

$$\psi^+(r) = e^{ikz} + \int d^3r'\, G_0^+(r-r')\, \langle r'|V|\psi^+\rangle \qquad (3d) \qquad (306)$$

so that, using (238), we have

$$\left.\begin{aligned} \psi_{scatt}(r) &= -\frac{2m}{\hbar^2}\int d^3r'\, \frac{e^{ik|r-r'|}}{4\pi|r-r'|}\, \langle r'|V|\psi^+\rangle \\ &\xrightarrow[kr \gg 1]{} -\frac{2m}{\hbar^2}\frac{1}{4\pi}\, T_{kk'}\, \frac{e^{ikr}}{r} \end{aligned}\right\} \quad (3d) \qquad (307)$$

and comparing with (201), we get

$$f_{kk'} = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\, T_{kk'} \qquad (308)$$

Now we notice that these relations look quite different from those in (294), which relate the partial wave components $f_l(k)$ to $t_l(k)$. This is because the $t_l(k)$ are actually matrix elements between energy eigenstates, instead of momentum eigenstates, and we need to transform between the two bases. Because we are running out of time I will not derive the results in (294) here.

BORN APPROXIMATION: Let us now look at what happens when we develop the integral eqtn for $T_{kk'}$ as a power series in $V_{kk'}$. The integral equation is most easily develop in k-space. As we saw in (221), we can write

$$\left.\begin{aligned} T_{kk'} &= V_{kk'} + \sum_{k''} V_{kk''}\, G_0^+(k'')\, T_{k''k'} \\ &= V_{kk'} + \sum_{k_1} V_{kk_1} G_0^+(k_1) V_{k_1k'} + \sum_{k_1}\sum_{k_2} V_{kk_1} G_0^+(k_1) V_{k_1k_2} G_0^+(k_2) V_{k_2k'} + \cdots \end{aligned}\right\} \qquad (309)$$

We can also write this series in a real space representation, viz.,

$$T_{kk'} = \int d^D r_1\, e^{i(\underline{k}-\underline{k}').\underline{r}_1} V(r_1) + \int d^D r_1 \int d^D r_2\, e^{i(k_1 r_1 - k_2 r_2)} V(r_1) G_0^+(\underline{r}_1 - \underline{r}_2) V(r_2) + \ldots \quad (310)$$

Now the 1st term in this expression is called the Born approximation - it is just the 1-time scattering off the potential, given by

$$T_{kk'}^{BORN} = V_{kk'} = \int d^D r\, e^{i(k-k').r} V(\underline{r}) \quad (311)$$

It is useful to work out explicit formulas for these in various dimensions. As already noted, in 3d we can write

$$V_{kk'} = \frac{4\pi}{|k-k'|} \int_0^\infty r\,dr\, V(r) \sin(|k-k'|r) \qquad (3d) \quad (312)$$

ie.,

$$V_k(\theta) = \frac{2\pi}{k \sin\theta/2} \int_0^\infty r\,dr\, V(r) \sin(2kr \sin\theta/2) \qquad (3d) \quad (313)$$

where the scattering angle θ is related to $|k-k'|$ by $|\underline{k}-\underline{k}'| = 2k \sin\theta/2$ (314)

In the same way we can write, in 2 dimensions

$$V_{kk'} = 2\pi \int_0^\infty r\,dr\, J_0(|k-k'|r) V(r) \qquad (2d) \quad (315)$$

and in 1d we have, letting $q = k-k'$

$$V_q = \int dx\, e^{iqx} V(x) \qquad (1d) \quad (314)$$

The Born approximation seems quite crude, and it is, but it can be useful under some circumstances, when the potential $V(r)$ can be treated as a small perturbation. To see formally when this is, we just compare the scattered wave with the incoming wave; if

$$|\Psi_{scatt}| \ll |e^{ik.r}| = 1 \quad (315)$$

then the Born approx. should be valid. Evaluating the scattered wave in the Born approximation, we have, for $kr \gg 1$:

$$\Psi_{scatt}^{Born} \longrightarrow \left\{ \begin{array}{lll} \frac{2m}{\hbar^2} \frac{-i}{2k} e^{ikx} V_{kk'} & \sim \frac{m}{\hbar^2 k} \bar{V} d_0 & (1d) \\ \frac{2m}{\hbar^2} \left(\frac{1}{8\pi k}\right)^{1/2} e^{i(kr+\pi/4)} \frac{V_{kk'}}{\sqrt{r}} & \sim \frac{m}{\hbar^2 k^{1/2}} \bar{V} d_0^{3/2} & (2d) \\ \frac{2m}{\hbar^2} \frac{-1}{4\pi} e^{ikr} \frac{V_{kk'}}{r} & \sim \frac{m}{\hbar^2} \bar{V} d_0^2 & (3d) \end{array} \right\} \quad (316)$$

where the quantity $\bar{V}$ is a typical value of the potential in the region of space where it is significant, over a length scale d_o - hence the total weight of the potential is given by

$$\int d^D r \; V(r) \sim \bar{V} d_o^D \qquad (317)$$

The results in (316) are very revealing: they tell us that in 3d, the Born approximation works provided the potential strength $\bar{V}$ is sufficiently small. In 3d, we can write

$$\text{If} \quad |\bar{V}| \ll \hbar^2/md_o^2 \equiv \bar{T} \quad \Longrightarrow \text{Born approx valid} \quad (3d) \qquad (318)$$

where we write $\bar{T}$ as the mean kinetic energy of a particle in the volume occupied by the potential, using the uncertainty principle. Notice an interesting consequence of this result, viz. that a weak 3d attractive potential can never give a bound state, because the perturbation Ψ_{scatt} on the original wave function is small (a bound state would necessarily involve a distortion of $\sim O(1)$ of the plane wave state at $k, E = 0$).

However in 2d or 1d the situation is very different - we see that as $k \to 0$, the Born approximation must break down. This is obvious from all the results we have so far for the functions $f_{kk'}$ and $T_{kk'}$. It is obvious in 1d from the form of the f-function in (299); every term diverges as $\sim 1/q$ as $q = k-k' \to 0$. In 2d the situation is a little more complicated, and we shall study it properly in the next sub-section.

UNITARITY & the OPTICAL THEOREM: Finally, in our study of scattering functions, let's return to the optical theorem and take a more general look at it.

We can summarise all our partial wave results as follows (with the α_k defined in (287)):

PARTIAL WAVE RELATIONS

- $$S_l(k) = e^{2i\delta_l(k)} = 1 + 2i\alpha_k f_l(k) \equiv 1 - 2it_l(k)$$
$$\equiv 1 + 2i e^{i\delta_l(k)} \sin\delta_l(k)$$

- $$f_l(k) = \frac{1}{\alpha_k} e^{i\delta_l(k)} \sin\delta_l(k) = \frac{1}{\alpha_k} \frac{1}{\cot\delta_l(k) - i} \equiv \frac{1}{g_l(k) - i\alpha_k}$$

- $$\mathrm{Im}\, f_l(k) = \frac{1}{\alpha_k}\sin^2\delta_l(k) \qquad \mathrm{Im}\, t_l(k) = -\sin^2\delta_l(k)$$

- $$|f_l(k)|^2 = 1/\alpha_k^2 \sin^2\delta_l(k) \qquad |t_l(k)|^2 = -\sin^2\delta_l(k)$$

- $$t_l(k) = -\alpha_k f_l(k) = \frac{1}{i - \cot\delta_l(k)} = -e^{i\delta_l(k)}\sin\delta_l(k)$$

- $$K_l(k) = -i\,\frac{1 - S_l(k)}{1 + S_l(k)} = -\tan\delta_l(k)$$

From this table we see that the simplest form in which we can write the optical theorem in the partial wave representation is just

$$\Im m\, t_l(k) = |t_l(k)|^2 \qquad (319)$$

which is equivalent to (287). Another way to write this is in terms of the T-matrix operator, on the energy shell, defined by eqtn (230). We then have

$$\Im m\, \hat{T}(E) = \pi |\hat{T}(E)|^2 \qquad (320)$$

We note that these results are a consequence of the relationship between the $S_l(k)$ and the $t_l(k)$ (and between $\hat{S}(E)$ and $\hat{T}(E)$), and the UNITARITY of the S-matrix.

$$|\hat{S}(E)| = |S_l(k)| = 1. \qquad (321)$$

Now all these relations are actually a simple consequence of the conservation of probability, ie., of particle conservation. We can see this in various ways. Note first that we define the S-matrix between initial and final states as

$$S_{fi} = \langle f|\hat{S}|i\rangle = \lim_{t\to\infty} \lim_{t'\to -\infty} \langle \psi_f(t)|\hat{G}(t,t')|\psi_i(t')\rangle \qquad (322)$$

where the initial & final states are chosen here to be incoming & outgoing waves; it then follows that, because

$$\hat{G}(t,t') = \exp\{-i/\hbar\, \hat{\mathcal{H}}(t_2,t_1)\} \qquad (323)$$

is a unitary operator, so must $\hat{S}$ be. Another way of seeing it is by arguing that the total particle conservation is expressed by

$$\partial_t |\psi|^2 + \nabla\cdot \underset{\sim}{j} = 0 \qquad (324)$$

and then calculating the flux $\int_\Omega dS\, \partial_t |\psi|^2 = \int_\Omega dS \cdot \underset{\sim}{j}(\underset{\sim}{r})$ (325)

across a surface far from the scatterer - because of angular momentum conservation for a spherically symmetric scatterer, probability conservation must hold for each partial wave. But we have already seen previously (cf eqtns (248) and (249)) that the only effect of scattering is to phase shift the outgoing waves with respect to incoming waves - this phase shift being described by the unitary function $S_l(k)$. The total flux of incoming & outgoing waves thus balance, so that the unitarity of $\hat{S}$ and of the $S_l(k)$ express the fact that there is no net flux through the surface.